

A note on the formal structure of quantum constrained systems

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The space of the solutions of Dirac's quantum constraints cannot be constructed factoring the quantum state space by the "simple" gauge transformations generated by the constraints. However, we show here that it can be constructed by factoring the state space by suitably defined "complete" gauge transformations. These are generated by the action of the quantum constraints on individual components of the quantum state.

I. INTRODUCTION

In classical mechanics, a gauge invariant state can be seen as an equivalence class of gauge noninvariant states. Two gauge noninvariant states are equivalent if there is a gauge transformation sending one into the other. The same fails to be true in quantum mechanics: Dirac's quantum constraints C generate the gauge transformation $\psi \rightarrow e^{itC}\psi$ on the quantum states, but physical states cannot be seen as equivalence classes under the equivalence relation

$$\psi \sim e^{itC}\psi. \quad (1)$$

Rather, physical states are the states which are annihilated by the Dirac constraints [1].

We show in this brief note that one can see physical states as equivalence classes of gauge noninvariant states in the quantum theory as well, but under an equivalence relation more complicated than (1). We call this alternative equivalence relation a "complete" quantum gauge transformation. Roughly, a complete quantum gauge transformation is defined as follows. $\phi \sim \psi$ iff there are states ρ_i and t_i 's such that

$$\begin{aligned} \psi &= \sum_i \rho_i \\ \phi &= \sum_i e^{it_i C} \rho_i. \end{aligned} \quad (2)$$

That is, a complete gauge transformation is obtained by independently gauge transforming linear components. We show below that the space of the solutions of Dirac's constraint is naturally identified with the space of the equivalence classes defined by this equivalence relation.

In general, in an infinite dimensional Hilbert space, the Dirac physical states can be generalized vectors that do not belong to the Hilbert space. In this case, the ρ_i in (2) may be generalized vectors as well. However, we shall show below that complete gauge equivalence can be defined in terms of the finite gauge operator e^{itC} also without recurring to generalized vectors. This fact allows us to construct the space of the physical states as a space of equivalence classes, without the need of extending the Hilbert space or using generalized vectors.

II. QUANTUM GAUGE TRANSFORMATIONS IN A FINITE DIMENSIONAL HILBERT SPACE

Let us assume that we have a unitary representation U of a group G in a Hilbert space \mathcal{H} . In this section we disregard all complications due to the infinite dimensionality of \mathcal{H} . The generators of the representation are the Dirac constraints, and the space of physical states \mathcal{H}_{Ph} is defined as the kernel of the Dirac constraints [1], namely as the trivial representation of G in \mathcal{H} . States in \mathcal{H}_{Ph} are gauge invariant, and represent physical states. A gauge noninvariant state can roughly be seen as a state in a particular gauge. Physical predictions of a classical gauge theory are given by gauge invariant quantities; but in concrete calculations, we usually employ a gauge-noninvariant description – leaving the task of extracting the physical quantities at the end. It would be nice to be able to do the same in the quantum theory, namely to work on \mathcal{H} without recurring to \mathcal{H}_{Ph} , keeping track of gauge equivalence.

The orthogonal projection π on \mathcal{H}_{Ph} provides the natural definition of quantum gauge equivalence in \mathcal{H} : $\phi \sim \psi$ iff

$$\pi(\phi) = \pi(\psi). \quad (3)$$

We have $\mathcal{H}_{Ph} = \underline{\mathcal{H}}$.

What is the precise relation between this equivalence and the transformations generated by U in \mathcal{H} ? Can we interpret this equivalence as the possibility of being gauge transformed, as we do for the quantum theory? More precisely, can we construct the equivalence relation \sim directly from U without having to solve for the invariant states first? Clearly if there exists a $g \in G$ such that

$$\phi = U[g]\psi \quad (4)$$

then $\phi \sim \psi$. However, the converse is not true in general. Namely ϕ and ψ can be gauge equivalent even if there is no $U[g]$ that maps one into the other.

To get some intuition on how this may come about consider the following simple example. Let the group $U(1)$ act on R^3 by generating rotations around the z axis. The invariant subspace is the one dimensional z axis, while the space of the orbits is the two dimensional space

of the circles parallel to the $z = 0$ plane and centered on the z axis.

Clearly, it is the linear structure of quantum mechanics that differentiates gauge equivalence from the fact of belonging to the same orbit: two orbits on the same $z = \text{constant}$ plan are in the same gauge equivalence class.

This example suggests that two quantum states are quantum gauge equivalent not only if they can be transformed into each other by a finite gauge transformation, but also if they can be decomposed into a linear combination of vectors which can be independently gauge transformed into each other. We make this intuition concrete as follows. We now show that ψ and ϕ are equivalent (that is (3) holds), iff there exist vectors $\rho_i \in \mathcal{H}$ and elements $g_i \in G$ such that

$$\begin{aligned}\psi &= \sum_i \rho_i, \\ \phi &= \sum_i U[g_i] \rho_i.\end{aligned}\tag{5}$$

To prove that (5) implies (3) is immediate: it suffices to notice that $\pi U[g] = \pi$ by definition. To prove the converse, we begin by proving that any vector ρ in the kernel K of π can be written as

$$\rho = \sum_i (U[g_i] \rho_i - \rho_i).\tag{6}$$

Let L be the space of all vectors that can be written as in (6). L is a linear subspace, it is left invariant by $U[g]$ and is contained in K . Let S be the subspace of K orthogonal to L . A vector ρ in S cannot be U invariant because it is in K , therefore $\chi = U[g]\rho - \rho$ is different from zero. But S must be left invariant as well, therefore $\chi \in S$ and not in L , but χ is also in L , by definition of L , therefore S is empty, $K = L$ and all vectors in K can be written as in (6).

Now, if $\pi(\phi) = \pi(\psi)$, then $(\phi - \psi) \in K$, therefore there are g_i and ρ_i such that

$$\phi - \psi = \sum_i (U[g_i] \rho_i - \rho_i).\tag{7}$$

It follows that

$$\phi - \sum_i U[g_i] \rho_i = \psi - \sum_i \rho_i \equiv \rho.\tag{8}$$

By adding ρ to both sums (with a corresponding $g = \text{identity}$), we have (5), *QED*.

Thus, if we *define* the following equivalence relation: $\phi \sim \psi$ iff there exist $\rho_i \in \mathcal{H}$ and $g_i \in G$ such that (5) holds – then we have

$$\mathcal{H}_{Ph} = \frac{\mathcal{H}}{\sim}.\tag{9}$$

Intuitively, a quantum state is a linear quantum superposition of classical configurations (a wave function over

configuration space). It is therefore reasonable that we may gauge transform each individual component of the superposition independently, without changing the gauge invariant quantum state.

We call the transformation $\psi \rightarrow U[g]\psi$ a “simple” quantum gauge transformation, and the transformation

$$\psi = \sum_i \rho_i \rightarrow \phi = \sum_i U[g_i] \rho_i\tag{10}$$

a “complete” quantum gauge transformation. We have proven that physical quantum states are not equivalence classes under simple quantum gauge transformations, but they are equivalence classes under complete quantum gauge transformations.

III. INFINITE DIMENSIONAL ISSUES

In infinite dimensional spaces, the well known infinitary subtleties of quantum mechanics appear. In general, zero can be in the continuum spectrum of the Dirac constraints and therefore physical states appear as generalized states. We have then to use continuum-spectrum techniques, such as Gelfand triples [2], or similar. In particular, \mathcal{H}_{Ph} is not a linear subspace of \mathcal{H} , but a linear subspace of a suitable closure $\overline{\mathcal{H}}$ of \mathcal{H} , which can be defined as the dual of a suitable dense subspace of \mathcal{H} .

In this case, the analysis of the previous section can be repeated with minor modifications, using $\overline{\mathcal{H}}$. U acts on $\overline{\mathcal{H}}$ by duality. \mathcal{H}_{Ph} is the U -invariant subspace of $\overline{\mathcal{H}}$. Let L be the subspace of $\overline{\mathcal{H}}$ formed by the vectors that can be written in the form (6), where now the sum may contain an infinite numbers of terms, and the required convergence is in $\overline{\mathcal{H}}$, not in \mathcal{H} . Consider $S = \frac{\overline{\mathcal{H}}}{\mathcal{H}_{Ph} \oplus L}$. As before, it is easy to see that S is linear and U -invariant. If ρ is a non vanishing vector in S , it cannot be U invariant (because it would be in \mathcal{H}_{Ph}) and $\chi = U[g]\rho - \rho$ is different from zero. But S is left invariant as well, therefore $\chi \in S$ and not in L , but χ is also in L , by definition of L , therefore S is empty and $\overline{\mathcal{H}} = \mathcal{H}_{Ph} \oplus L$.

Notice that even if ψ and ϕ are in \mathcal{H} , in general the ρ_i 's are in $\overline{\mathcal{H}}$ and not in \mathcal{H} . More precisely, the r.h.s. of (7) is obviously in \mathcal{H} if ψ and ϕ are; but when we split the sum into the two sums in (8), the individual sums need not converge in \mathcal{H} . Thus, ρ in (8) may be a generalized vector. Therefore we can still define \mathcal{H}_{Ph} as the space of the equivalence classes of vectors in \mathcal{H} under the equivalence relation (5), but we must allow for decompositions in generalized vectors ρ_i as well.

However, the analysis above suggests that we can avoid the cumbersome introduction of $\overline{\mathcal{H}}$ and generalized vectors altogether. This follows from the fact that space L of the vectors that can be written in the form (6) is a proper subspace of \mathcal{H} . Thus, we can define L first, and construct the linear space \mathcal{H}_{Ph} as the space of the equivalence classes of vectors in \mathcal{H} , equivalent under the addition of vectors in L , namely as $\frac{\mathcal{H}}{L}$. In other words,

we can define the equivalence relation by (7) instead than by (5). This is done as follows.

Given an infinite dimensional Hilbert space \mathcal{H} and a unitary representation U of a group G over it, we define L as the closed linear subspace of \mathcal{H} formed by the vectors that can be written as

$$\rho = \sum_{i=1}^{\infty} (U[g_i] \rho_i - \rho_i). \quad (11)$$

We then call two states gauge equivalent if their difference is in L , and define

$$\mathcal{H}_{Ph} = \frac{\mathcal{H}}{L}. \quad (12)$$

The space \mathcal{H}_{Ph} is defined in this way without recurring to generalized vectors or other extensions of \mathcal{H} . This space is naturally isomorphic to the space of generalized vectors that solve the Dirac constraints.

To clarify how this may happen, consider the following. In finite dimensions, if L is a proper subspace of \mathcal{H} , then L_{\perp} the orthogonal complement of L (that is, the set of vectors orthogonal to L) is nontrivial, and

$$\mathcal{H} = L_{\perp} \oplus L. \quad (13)$$

We can thus identify L_{\perp} with $\frac{\mathcal{H}}{L}$. In infinite dimensions, the orthogonal complement L_{\perp} of a subspace L may be trivial (contain only the zero vector) even if L is smaller than \mathcal{H} . But $\frac{\mathcal{H}}{L}$ exists nevertheless, and it is naturally identifiable with the space of *generalized* vectors perpendicular to L . Gauge invariance of a generalized vector means being perpendicular to L . Therefore, if we construct \mathcal{H}_{Ph} by requiring gauge invariance (solving the Dirac constraints), we need generalized vectors. But if we construct \mathcal{H}_{Ph} as the space of the gauge equivalence classes, we do not need to introduce generalized states.

IV. A SIMPLE EXAMPLE

Let us see how this is realized in a very simple example. Let \mathcal{H} be the space $L_2[R^2]$ of functions $\psi(x, y)$, and let us have a single constraint $C = i \frac{\partial}{\partial y}$. The group G is the abelian group R that acts on \mathcal{H} by displacing functions in the y direction: $U(a)\psi(x, y) = \psi(x, y + a)$. What is the space L ? All the vectors of the form $\rho = U(a)\psi - \psi$ satisfy

$$\int dy \rho(x, y) = 0, \quad (14)$$

and any vector that satisfies (14) can be approximated in norm by a sequence of vectors of the form $\rho = U(a)\psi - \psi$. Therefore equation (14) defines the subspace L in \mathcal{H} . Notice that L is a well defined proper subspace of \mathcal{H} . According to our definition, two functions $\psi(x, y)$ and

$\phi(x, y)$ are gauge equivalent if their difference is in L , namely if

$$\int dy (\psi(x, y) - \phi(x, y)) = 0. \quad (15)$$

We can characterize (a dense subspace of) the equivalence classes by functions of one variable

$$\psi(x) \equiv \int dy \psi(x, y) = \int dy \phi(x, y). \quad (16)$$

Therefore the map $\pi : \mathcal{H} \mapsto \mathcal{H}_{Ph}$ is integration in dy and \mathcal{H}_{Ph} is formed by square integrable functions of x alone.*

A “simple” gauge transformation is a rigid displacement of $\psi(x, y)$ along the y axis. A “complete” gauge transformation is the addition of any function with vanishing $\int dy$ integral. The physical space is the space of the functions $\psi(x, y)$ modulo these complete gauge transformations.

V. CONCLUSIONS

We have introduced the notion of complete quantum gauge transformation. In the finite dimensional case, a complete gauge transformation is obtained by decomposing a vector in components and acting with the exponentiated constraints on each component independently. Namely, two vectors are gauge equivalent if equation (5) holds. In the infinite dimensional case, the same can be done allowing decompositions on bases of generalized vectors as well. Equivalently, two states ψ and ϕ are quantum gauge equivalent if their difference is in the closure of the space of the linear combinations of the vectors $U(g)\psi - \psi$, namely if (7) holds. Using this second strategy, there is no need of introducing generalized vectors. Dirac’s physical state space \mathcal{H}_{Ph} can be obtained as the space of the equivalence classes of states, under complete quantum gauge transformations.

In the classical hamiltonian theory of constrained systems, one has to take two steps in order to reduce the full phase space Γ to the physical phase space Γ_{Ph} . First, solve the constraint; that is, find the constraint surface C in Γ . Second, factor away the gauge transformation; that is, define Γ_{Ph} as the space of the gauge orbits in C . Dirac showed that in the quantum theory a single step is sufficient: the physical states are the ones that solve the

*We recall that, contrary to what often stated, \mathcal{H} naturally induces a scalar product in \mathcal{H}_{Ph} , although some work may be required to write this scalar product explicitly. In the present example, for instance, a spectral decomposition theorem states that \mathcal{H} can be written as a direct integral of Hilbert spaces $\mathcal{H} = \int dk \mathcal{H}_k$ [3]. C is diagonal in each \mathcal{H}_k with eigenvalue k . The point here is that \mathcal{H}_0 is naturally identified with \mathcal{H}_{Ph} , and it carries a scalar product.

quantum constraints. Here we have shown that one can take this single step also by factoring away (complete) quantum gauge transformations. Thus, in the classical theory we find the physical states by solving the constraints *and* factoring away the gauge transformations. In the quantum theory we find the physical states by solving the constraints *or* factoring away the gauge transformations.

The existence of this alternative strategy for dealing with quantum constraints is of some interest by itself, as a small further clarification of the structure of constrained quantum systems. But it might also have some practical application. First, it may allow us to avoid the cumbersome use of generalized vectors or extensions of the Hilbert space, as illustrated in sections III and IV. (Techniques for explicitly constructing the scalar product in the physical Hilbert space are still required, however.) Second, there are systems in which the Dirac operator is ill defined, but its exponentiated action is well defined. A typical example is the diffeomorphism constraint in loop quantum gravity (see [4] and references therein). In these cases, finite gauge transformations are very natural objects in the quantum theory. Finally, when the physical state space is too complicated to be constructed explicitly, the above construction opens the possibility of working with gauge noninvariant states without losing track of gauge equivalence. In loop quantum gravity, steps towards the construction of the exponentiated hamiltonian constraint operator have been taken [5]. An orbit generated by this operator corresponds to the coordinate-time evolution of a quantum states of gravity, or to a “quantum spacetime”. This note may help clarifying its physical interpretation. These applications will be discussed elsewhere.

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